

Isophthalic acid, 4-methylpent-2-yl octyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C22H34O4/c1-5-6-7-8-9-10-14-25-21(23)19-12-11-13-20(16-19)22(24)26-18(4 |
| InchiKey: | UPCGEBZTOLFCRT-UHFFFAOYSA-N |
| Formula: | C22H34O4 |
| SMILES: | CCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1 |
| Mol. weight [g/mol]: | 362.50 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -235.58 | kJ/mol | Joback Method |
| hf | -772.51 | kJ/mol | Joback Method |
| hfus | 44.92 | kJ/mol | Joback Method |
| hvap | 85.04 | kJ/mol | Joback Method |
| log10ws | -6.85 | | Crippen Method |
| logp | 5.795 | | Crippen Method |
| mcvol | 311.960 | ml/mol | McGowan Method |
| pc | 1184.16 | kPa | Joback Method |
| rinpol | 2501.00 | | NIST Webbook |
| tb | 886.12 | K | Joback Method |
| tc | 1091.62 | K | Joback Method |
| tf | 490.96 | K | Joback Method |
| vc | 1.196 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 998.25 | J/molxK | 886.12 | Joback Method |
| cpg | 1014.95 | J/molxK | 920.37 | Joback Method |
| cpg | 1030.37 | J/molxK | 954.62 | Joback Method |
| cpg | 1044.54 | J/molxK | 988.87 | Joback Method |
| cpg | 1057.48 | J/molxK | 1023.12 | Joback Method |
| cpg | 1069.24 | J/molxK | 1057.37 | Joback Method |
| cpg | 1079.83 | J/molxK | 1091.62 | Joback Method |
| dvisc | 0.0006178 | Paxs | 490.96 | Joback Method |
| dvisc | 0.0002874 | Paxs | 556.82 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001572 | Paxs | 622.68 | Joback Method |
| dvisc | 0.0000965 | Paxs | 688.54 | Joback Method |
| dvisc | 0.0000645 | Paxs | 754.40 | Joback Method |
| dvisc | 0.0000460 | Paxs | 820.26 | Joback Method |
| dvisc | 0.0000345 | Paxs | 886.12 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U356445&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/52-377-6/Isophthalic-acid-4-methylpent-2-yl-octyl-ester.pdf>

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